GEORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ______

Project No. G-35-608 R5899-0A0 — GTRI/~~GIT~~ — DATE 2 / 19 / 85

Project Director: Dr. C. S. Kiang — School/~~Lab~~ Geo Sciences

Sponsor: NASA Headquarters, Washington, DC 20546

Type Agreement: Grant No. NAGW-698

Award Period: From 1/1/85 To 12/31/85 (Performance) 12/31/85 (Reports)

Sponsor Amount:

	This Change	Total to Date
Estimated:	$	$
Funded:	$ 53,279	$ 53,279

Cost Sharing Amount: $ 16,746 — Cost Sharing No: G-35-323

Title: Theoretical Studies of the Chemical, Microphysical, and Dynamical Effects of Volcanic Intermissions on the Stratosphere.

ADMINISTRATIVE DATA

OCA Contact R. Dennis Farmer X4820

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Defense Priority Rating: ______

Military Security Classification: ______

(or) Company/Industrial Proprietary: ______

RESTRICTIONS

See Attached NASA Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval – Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with GIT

COMMENTS:

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Project Director	Procurement/EES Supply Services	GTRI
Research Administrative Network	~~Research Security Services~~	Library
Research Property Management	Reports Coordinator (OCA)	Project File
Accounting	Research Communications (2)	Other Jones

FORM OCA 4:383

GEORGIA INSTITUTE OF TECHNOLOGY
OFFICE OF CONTRACT ADMINISTRATION

NOTICE OF PROJECT CLOSEOUT

Closeout Notice Date 08/02/91

Project No. G-35-608 Center No. R5899-0A0

Project Director KIANG C S School/Lab E & A SCI

Sponsor NASA/HEADQUARTERS/WASHINGTON, DC

Contract/Grant No. NAGW-698 Contract Entity GTRC

Prime Contract No.

Title THEORETICAL STUDIES OF THE CHEMICAL, MICROPHYSICAL ANDDYNAMIC .....STRATO

Effective Completion Date 871231 (Performance) 871231 (Reports)

Closeout Actions Required:	Y/N	Date Submitted
Final Invoice or Copy of Final Invoice	Y	891115
Final Report of Inventions and/or Subcontracts	Y	880229
Government Property Inventory & Related Certificate	Y	
Classified Material Certificate	N	
Release and Assignment	Y	891115
Other	N	

Comments

Subproject Under Main Project No.

Continues Project No.

Distribution Required:

Project Director	Y
Administrative Network Representative	Y
GTRI Accounting/Grants and Contracts	Y
Procurement/Supply Services	Y
Research Property Managment	Y
Research Security Services	N
Reports Coordinator (OCA)	Y
GTRC	Y
Project File	Y
Other	N
	N

NOTE: Final Patent Questionnaire sent to PDPI.

Georgia Institute of Technology
A UNIT OF THE UNIVERSITY SYSTEM OF GEORGIA
ATLANTA, GEORGIA 30332
SCHOOL OF GEOPHYSICAL SCIENCES
404/894-3893

14 March 1988

Sponsor's I.D. No. - 02 105 002 87 008

Ms. Cherie Mockler
Grants Specialist
NASA Headquarters
CODE HWC/Contracts and Grants
Washington, D.C. 20546

Dear Ms. Mockler:

Attached hereto please find the progress report of "Theoretical Studies of the Chemical, Microphysical and Dynamic Effects of Volcanic Intrusions on the Stratosphere". Though direct funding for the project has ended, the authors request that a limited amount of additional funding be made available to allow for costs associated with finishing up the project. These costs involve funding for the student who has done the work and is in the process of initiating the writing of the final document, a small amount of computer funding associated with producing it (text, plots, tables, etc.), and support for carrying out the necessary tasks of reproduction of extra copies of the report, etc.

Your consideration of this request will be appreciated. If you think it is possible, please let me know about the limitation.

Thanking you in advance, I remain,

Sincerely,

C. S. Kiang, Director and
Project Director
SCHOOL OF GEOPHYSICAL SCIENCES

CSK:rb
encl.
cc: Dean Karlovitz
OCA

Project No. - G-35-608

PROGRESS REPORT

This report summarizes the essential elements of and progress on the grant entitled: " Theoretical Studies of the Chemical, Microphysical and Dynamic Effects of Volcanic Intrusions on the Stratosphere".

The purpose of the study was to address some of the difficulties associated with initiating multidimensional models for use in studying the effects associated with introduction of large quantities of ash and gases into the background stratosphere from volcanic sources. A number of interesting processes take place at short times after the eruption which can not be adequately handled by a larger, computationally bound code. It was hoped that this project would provide a more detailed picture of what goes on during the first few weeks between the initial eruption and the time the volcanic cloud reaches global proportion. The initial intent was to apply the model to the case of the April 1982 eruption of El Chichon. We have also applied the model in studying the effects of the Mt. St. Helens eruption of May 18, 1980.

As originally proposed, we intended to treat the cloud as a single entity whose concentration profile (gas and ash) was gaussian in all three spatial dimensions. Within that cloud, the sulfur-bearing gasses would oxidize to form sulfuric acid vapor which would then condense on the ash particles, which also would undergo coagulation with each other. It was realized very shortly thereafter, however, that sedimentation would invalidate the single plume model. The gases and small particles would reside in the originally deposited layer during the entire transit of the globe, but the larger particles would continue to separate from it. Hence, condensation and coagulation would become increasingly less important for particles which become furthest separated from the main plume, i.e., the larger particles. In order to account for this, we developed a new scheme in which a series of discrete particle sizes would each be represented by a separate plume, also gaussian, which would be allowed to independently interact with each other as well as be differentially transported and dispersed by the winds.

This necessarily made the model more computationally complex, but the assumed gaussian spatial symmetry of the plumes which represent the overall volcanic cloud made the work much easier. In making this assumption, we gave up the ability to do certain things. For instance, when condensation and coagulation occur at the edges of partially overlapping plumes, an asymmetry would naturally develop that would partly destroy the gaussian spatial symmetry. The function which describes the particle number densities is expressed as the product of a radial distribution function and three gaussian spatial functions. The mathematical averaging of the physical processes in the overlap region of interest folds this asymmetry into the radial function. This is not a significant error for two reasons. First, the gaussian widths are almost totally controlled by large scale dispersion in the atmosphere. Secondly, most of the particle growth takes place at particle sizes which do not rapidly sediment during the global transit. Hence, this approximation will not affect any of the major conclusions derived from the model.

Another consideration which we had to face in performing the coagulation calculations involved locating the position of and determining the properties of "phantom plumes". Gas-to-particle conversion occurs in the region of overlap between the gas cloud and each particle cloud. Coagulation involves summing the contributions from all two particle combinations whose size adds up to the radius of a particular plume. Hence, one must know the number density, position and gaussian widths of plumes which do not occur at the discrete sizes chosen for the computation. It is not a serious problem, but does require interpolating between plume sizes.

One of the important scientific questions that we wanted to answer was whether or not it was possible for the model to predict new particle formation. Although the theory of nucleation has inherent limitations in practical use, experimental observations suggest that certain levels of sulfuric acid vapor are required for nucleation to take place. Hence, a photochemical model in which the concentrations of key species such as ozone, water vapor, hydroxyl radicals, etc., are allowed to vary as the plumes impact on them is necessary. Such a sub-model has been constructed and we find, in fact, that there are realistic assumed initial conditions in which it is possible to generate enough sulfuric acid vapor to cause nucleation to occur. Hence, a parameterization was developed which allows us to roughly simulate the production of new particles. The implications of this will be discussed in the final report.

As of the writing of this report, the El Chichon results have been completed and are undergoing analysis. The results for Mt. St. Helens have already begun. The final report to NASA should be available by the end of June. In the interim, the student who is preparing the report will be completing the mathematical formulation of the model for his thesis, and it can be made available if necessary within a few weeks.

10 March 1988

WORK STATEMENT

The following represents a summary of the work completed to date, followed by an analysis of the remaining work yet to be performed for the grant entitled "Theoretical Studies of the Chemical, Microphysical and Dynamic Effects of Volcanic Intrusions", (NASA Grant NAGW-698). We proposed to develop and test a theoretical model to be applied in the study of the effects of volcanic injections of trace gases and particulate matter on the stratosphere. A Lagrangian plume model, to simulate the chemical and microphysical effects caused from the time of initial injection, until the plume encircled the globe is proposed to provide a better initial simulation of volcanic eruption. The output from this model would then be used as input to a 2-D model which would extend the simulation to global dimensions. The two coupled models would then be used to simulate the eruption, in early April of 1982, of El Chichon.

The Lagrangian plume model, as originally proposed, consisted of three basic subsections, namely (1) A transport algorithm, which computes the motion of the center of the plume and estimates the rate of plume dispersion due to local variables such as the wind direction, wind shear, static stability, etc., (2) A photochemical algorithm, which computes the rates of relevant gas phase chemical processes, especially those which lead to formation of sulfuric acid aerosols, and (3) An aerosol physics package which treats the microphysical processes involved in gas-to-particle conversion, as well as coagulation and sedimentation.

After submission of the proposal, and prior to its acceptance by NASA, it was discovered that differential sedimentation of the larger particles in the volcanic cloud would destroy the assumed Gaussian symmetry of the plume. Each large particle size "bin" would become, in effect, a new plume, separate from the original one. To account for this effect, we decided to treat those size categories which separate sufficiently from the main plume, on time scales comparable to that required to circle the globe, as separate plumes. Wind shear will cause horizontal separation of the plume centers, but chemical and microphysical effects will still occur in the regions of plume overlap. This will, potentially, distort the spatial symmetry of each plume. Hence, the perturbations to each plume must be assessed. After each time step, the plumes will be renormalized. The composition of the entire volcanic cloud will, thus, be represented by the sum of the individual plumes.

The majority of the time utilized thus far has been spent upon devising a method for treating plume fractionation and renormalization. The photochemical portion of the model is completed. Currently, any of the reactions which are contained within the latest NASA/JPL rate constant assessment may be selected. The subroutines contained therein are called by the same integrator which handles the aerosol physics. The aerosol routines are complete (except for merging them into the entire package), and are set up to handle nucleation, condensation/evaporation, coagulation and sedimentation. The current form of the transport algorithm utilizes mean properties of the atmosphere for the season in question. The dispersion rates are computed as described in the original proposal. Hence, all that remains to be done is to complete the algorithm for renormalizing the plume and merging all the subroutines together as a package. We estimate that six (6) months will be required to complete this process, and to generate final results. The initial form of the 2-D will employ has already been written and tested, as described in the original proposal. It will, however, need to be adapted for use on either the campus CYBER 855 or the CYBER 205 located at the University of Georgia, in Athens, Georgia. We believe that within six (6) months we will be able to obtain first results from this model which couples the Lagrangian plume model with existing 2-D transport and chemical and microphysical model.